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## *N,N'*-Bis(pyridin-3-yl)oxamide

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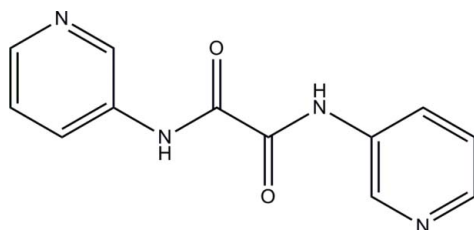
Received 12 March 2013; accepted 17 March 2013

Key indicators: single-crystal X-ray study;  $T = 297$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.043;  $wR$  factor = 0.126; data-to-parameter ratio = 12.8.

The title molecule,  $\text{C}_{12}\text{H}_{10}\text{N}_4\text{O}_2$ , located about an inversion centre, is roughly planar, with an r.m.s. deviation from the least-squares plane of all non-H atoms of 0.019 Å. In the crystal,  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds between the amide  $\text{N}-\text{H}$  group and the pyridine N atom connect the molecules into a corrugated layer parallel to  $(10\bar{1})$ .

## Related literature

For *N,N'*-di(3-pyridyl)oxamide and its metal complexes, see: Hu *et al.* (2012).



## Experimental

### Crystal data

$\text{C}_{12}\text{H}_{10}\text{N}_4\text{O}_2$

$M_r = 242.24$

Monoclinic,  $P2_1/n$   
 $a = 3.8992$  (7) Å  
 $b = 12.662$  (2) Å  
 $c = 10.9678$  (17) Å  
 $\beta = 97.983$  (4)°  
 $V = 536.26$  (16) Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 297$  K  
 $0.58 \times 0.20 \times 0.06$  mm

### Data collection

Bruker SMART 1000  
diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 1997)  
 $T_{\min} = 1.000$ ,  $T_{\max} = 1.000$

2997 measured reflections  
1050 independent reflections  
768 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.126$   
 $S = 1.06$   
1050 reflections

82 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.26$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{N2}^i$	0.86	2.26	3.061 (2)	156

Symmetry code: (i)  $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the National Science Council of the Republic of China for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2563).

## References

- Bruker (1997). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Hu, H.-L., Hsu, Y.-F., Wu, C.-J., Yeh, C.-W., Chen, J.-D. & Wang, J.-C. (2012). *Polyhedron*, **33**, 280–288.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supplementary materials

*Acta Cryst.* (2013). E69, o560 [doi:10.1107/S1600536813007277]

***N,N'*-Bis(pyridin-3-yl)oxamide**

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**Comment**

Several Zn(II), Cd(II) and Hg(II) complexes containing *N,N'*-di(3-pyridyl)oxamide ligands have been reported, which show one-dimensional chains and metallocycles (Hu *et al.*, 2012). Within this project the crystal structure of the title compound was determined (Fig. 1). In its crystal structure intermolecular N—H···N hydrogen bonds are found (Table 1 & Fig. 2).

**Experimental**

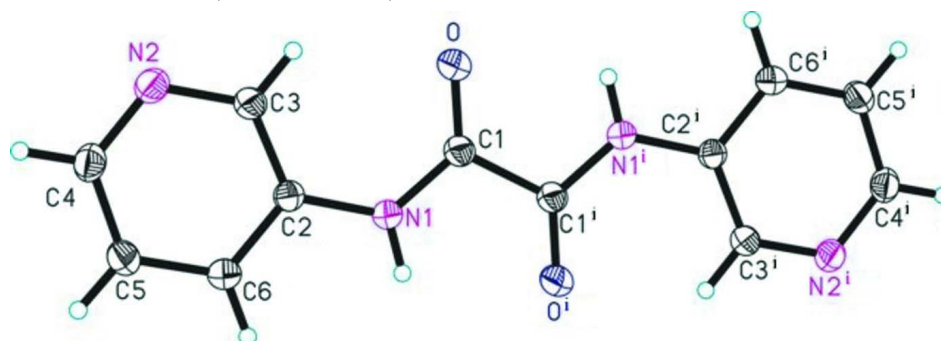
The title compound was prepared according to a published procedure (Hu *et al.*, 2012). Block crystals suitable for X-ray crystallography were obtained by slow evaporation of the solvent from a solution of the title compound in methanol.

**Refinement**

H atoms bound to C and N atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and N—H = 0.86 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5 U_{\text{eq}}(\text{C/N})$ .

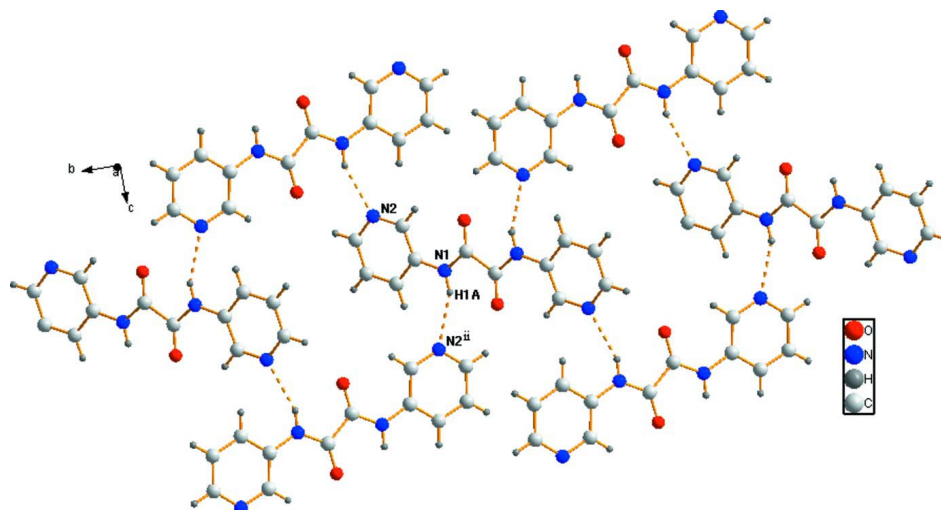
**Computing details**

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997) and *SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).



**Figure 1**

Molecular structure of the title compound with atom labeling and displacement ellipsoids drawn at the 30% probability level.



**Figure 2**

Hydrogen bonding interactions in the title compound.

### *N,N'*-Bis(pyridin-3-yl)oxamide

#### *Crystal data*

$C_{12}H_{10}N_4O_2$   
 $M_r = 242.24$   
 Monoclinic,  $P2_1/n$   
 Hall symbol:  $-P\ 2_1n$   
 $a = 3.8992\ (7)\ \text{\AA}$   
 $b = 12.662\ (2)\ \text{\AA}$   
 $c = 10.9678\ (17)\ \text{\AA}$   
 $\beta = 97.983\ (4)^\circ$   
 $V = 536.26\ (16)\ \text{\AA}^3$   
 $Z = 2$

$F(000) = 252$   
 $D_x = 1.500\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 1108 reflections  
 $\theta = 2.5\text{--}25.6^\circ$   
 $\mu = 0.11\ \text{mm}^{-1}$   
 $T = 297\ \text{K}$   
 Parallelepiped, colorless  
 $0.58 \times 0.20 \times 0.06\ \text{mm}$

#### *Data collection*

Bruker SMART 1000  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (*SADABS*; Bruker, 1997)  
 $T_{\min} = 1.000$ ,  $T_{\max} = 1.000$

2997 measured reflections  
 1050 independent reflections  
 768 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$   
 $\theta_{\max} = 26.0^\circ$ ,  $\theta_{\min} = 2.5^\circ$   
 $h = -4 \rightarrow 4$   
 $k = -15 \rightarrow 14$   
 $l = -12 \rightarrow 13$

#### *Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.126$   
 $S = 1.06$   
 1050 reflections  
 82 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.075P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.19\ \text{e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26\ \text{e \AA}^{-3}$

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O	0.1096 (4)	0.96926 (10)	1.15577 (12)	0.0530 (5)
N1	0.2264 (4)	0.87848 (10)	0.98550 (13)	0.0342 (4)
H1A	0.2033	0.8827	0.9065	0.041*
N2	0.6079 (4)	0.67892 (12)	1.21174 (13)	0.0421 (5)
C1	0.0929 (5)	0.95887 (12)	1.04473 (16)	0.0344 (4)
C2	0.3993 (4)	0.78835 (13)	1.03865 (15)	0.0309 (4)
C3	0.4530 (5)	0.76739 (14)	1.16394 (16)	0.0382 (5)
H3A	0.3784	0.8168	1.2173	0.046*
C4	0.7184 (5)	0.60928 (14)	1.13512 (17)	0.0416 (5)
H4A	0.8238	0.5476	1.1676	0.050*
C5	0.6832 (5)	0.62458 (14)	1.00998 (17)	0.0404 (5)
H5A	0.7667	0.5747	0.9593	0.048*
C6	0.5223 (5)	0.71506 (13)	0.96066 (16)	0.0367 (5)
H6A	0.4964	0.7269	0.8762	0.044*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O	0.0796 (11)	0.0451 (9)	0.0339 (8)	0.0183 (7)	0.0064 (7)	−0.0030 (6)
N1	0.0433 (9)	0.0310 (8)	0.0283 (8)	0.0024 (6)	0.0057 (6)	0.0002 (6)
N2	0.0547 (11)	0.0349 (9)	0.0351 (9)	−0.0016 (7)	0.0012 (7)	0.0017 (7)
C1	0.0387 (10)	0.0312 (9)	0.0337 (9)	−0.0020 (7)	0.0065 (7)	−0.0017 (7)
C2	0.0339 (9)	0.0277 (8)	0.0313 (9)	−0.0046 (7)	0.0048 (7)	−0.0007 (7)
C3	0.0501 (12)	0.0311 (9)	0.0335 (10)	−0.0017 (7)	0.0066 (8)	−0.0028 (8)
C4	0.0479 (11)	0.0324 (9)	0.0428 (11)	0.0021 (8)	0.0001 (8)	0.0030 (8)
C5	0.0446 (11)	0.0354 (10)	0.0411 (10)	0.0039 (8)	0.0061 (8)	−0.0042 (8)
C6	0.0416 (11)	0.0380 (10)	0.0305 (9)	0.0014 (8)	0.0050 (7)	−0.0009 (8)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

O—C1	1.218 (2)	C2—C6	1.392 (2)
N1—C1	1.350 (2)	C3—H3A	0.9300
N1—C2	1.410 (2)	C4—C5	1.374 (3)
N1—H1A	0.8600	C4—H4A	0.9300
N2—C4	1.330 (2)	C5—C6	1.380 (2)
N2—C3	1.344 (2)	C5—H5A	0.9300
C1—C1 <sup>i</sup>	1.541 (3)	C6—H6A	0.9300

C2—C3	1.387 (2)		
C1—N1—C2	127.27 (14)	N2—C3—H3A	118.5
C1—N1—H1A	116.4	C2—C3—H3A	118.5
C2—N1—H1A	116.4	N2—C4—C5	122.78 (17)
C4—N2—C3	118.26 (15)	N2—C4—H4A	118.6
O—C1—N1	126.31 (16)	C5—C4—H4A	118.6
O—C1—C1 <sup>i</sup>	121.25 (19)	C4—C5—C6	119.04 (17)
N1—C1—C1 <sup>i</sup>	112.44 (17)	C4—C5—H5A	120.5
C3—C2—C6	117.65 (16)	C6—C5—H5A	120.5
C3—C2—N1	124.21 (15)	C5—C6—C2	119.30 (16)
C6—C2—N1	118.14 (14)	C5—C6—H6A	120.3
N2—C3—C2	122.94 (16)	C2—C6—H6A	120.3

Symmetry code: (i)  $-x, -y+2, -z+2$ .

*Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )*

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ N2 <sup>ii</sup>	0.86	2.26	3.061 (2)	156

Symmetry code: (ii)  $x-1/2, -y+3/2, z-1/2$ .